

John E. Klepeis

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Citizenship: USA
Position: Theoretical condensed matter physicist

Educational Background

1989 Ph. D. in Applied Physics, Stanford University, Stanford, CA

1987 M. S. in Applied Physics, Stanford University, Stanford, CA

1985 B. S. in Applied and Engineering Physics, Cornell University, Ithaca, N. Y.

Employment Experience

1989–present

Theoretical condensed matter physicist, Lawrence Livermore National Laboratory, Livermore, CA; Application of first principles computational methods to the electronic structure of surfaces and interfaces, semiconductors, wide bandgap insulators, and materials at high pressure; Close collaborations with experimentalists; Supervise summer students; Write research proposals; Manage research programs; Promoted to term appointment, 9/92; Promoted to career appointment, 4/96.

Fall 1991/Temporary

Visiting scientist, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; Invited for 3 month visit; Studied metals on GaAs (110) surface; Acquired expertise with an advanced electronic structure method from author of the code.

1985–1989/Graduate Study

Graduate research assistant in Applied Physics, Stanford University, Stanford, CA; Semi-empirical tight-binding electronic structure calculations for semiconductor systems; Substitute lecturing; Tutored students; Graded problem sets.

Professional Affiliations and Honors

Member of the American Physical Society

Elected into Tau Beta Pi (1984) and Phi Kappa Phi (1985) Honor Societies, Cornell University

Publications

- J. E. Klepeis and W. A. Harrison, *Core electron binding energy shifts and screening in tetrahedral semiconductors*, J. Vac. Sci. Technol. B **5**, 1250 (1987).
- W. A. Harrison and J. E. Klepeis, *Dielectric screening in semiconductors*, Phys. Rev. B **37**, 864 (1988).
- J. E. Klepeis and W. A. Harrison, *Electronic structure of small coverages of column III metals on silicon (100)*, J. Vac. Sci. Technol. B **6**, 1315 (1988).
- J. E. Klepeis and W. A. Harrison, *Coverage dependence of Schottky barrier formation*, J. Vac. Sci. Technol. B **7**, 964 (1989).
- J. E. Klepeis and W. A. Harrison, *Charge-state-dependent atomic geometries for isolated metal adatoms on GaAs(110)*, Phys. Rev. B **40**, 5810 (1989).
- J. E. Klepeis, *Self-consistent electronic structure of semiconductor systems*, Unpublished Ph. D. thesis, Stanford University, Stanford, CA, 1989.
- J. E. Klepeis, K. J. Schafer, T. W. Barbee III, and M. Ross, *Hydrogen-Helium mixtures at megabar pressures: Implications for Jupiter and Saturn*, Science **254**, 986 (1991).
- J. E. Klepeis, C. Mailhiot, M. van Schilfgaarde, and M. Methfessel, *Role of ionicity in the determination of surface atomic geometries: GaP, ZnS, and CuCl (110) surfaces*, J. Vac. Sci. Technol. B **11**, 1463 (1993).
- A. K. McMahan, J. E. Klepeis, M. van Schilfgaarde, and M. Methfessel, *Bonding in the molybdenum silicides*, Phys. Rev. B **50**, 10 742 (1994).
- D. B. Boercker, J. E. Klepeis, and C. J. Wu, *Toward improved understanding of material surfaces and interfaces*, Energy and Technology Review, p. 25, August–September, 1994.
- J. E. Klepeis, E. L. Shirley, and M. P. Surh, *Predicting the structural and electronic properties of scintillators*, Energy and Technology Review, p. 33, August–September, 1994.
- T. Kendelewicz, J. E. Klepeis, J. C. Woicik, S. H. Southworth, C. Mailhiot, M. van Schilfgaarde, M. Methfessel, A. Herrera-Gomez, and K. E. Miyano, *Large-angle bond-rotation relaxation for CdTe (110)*, Phys. Rev. B **51**, 10 774 (1995).
- C. J. Wu, L. H. Yang, J. E. Klepeis, and C. Mailhiot, *Ab initio pseudopotential calculations of the atomic and electronic structure of the Ta (100) and (110) surfaces*, Phys. Rev. B **52**, 11 784 (1995).

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- J. E. Klepeis, L. J. Terminello, and D. A. Lapiano-Smith, *Imaging of a surface state from clean Cu (001)*, Phys. Rev. B **53**, 16 035 (1996).
- C. J. Wu and J. E. Klepeis, *Halogen adsorption on transition-metal surfaces: A case study of Cl on Ta(110)*, Phys. Rev. B **55**, 10 848 (1997).
- H. E. Lorenzana, J. E. Klepeis, M. J. Lipp, W. J. Evans, H. B. Radousky, and M. van Schilfgaarde, *High-pressure phases of PbF₂: A joint experimental and theoretical study*, Phys. Rev. B **56**, 543 (1997).
- T. W. Barbee III, A. K. McMahan, J. E. Klepeis, and M. van Schilfgaarde, *High-pressure boron hydride phases*, Phys. Rev. B **56**, 5148 (1997).
- A. K. McMahan and J. E. Klepeis, *Direct calculation of Slater-Koster parameters: Fourfold-coordinated silicon/boron phases*, Phys. Rev. B **56**, 12 250 (1997).
- A. K. McMahan and J. E. Klepeis, *Ab initio calculation of tight-binding parameters*, in Mat. Res. Soc. Symp. Proc. Vol. 491, edited by P. E. A. Turchi, A. Gonis, and L. Colombo (Materials Research Society, Warrendale, PA, 1998), p. 199.
- C. J. Wu and J. E. Klepeis, *The effect of Cl coverage on Si(100) surface reactivity: Implications for Cl etching of Si*, J. Phys.: Condens. Matter **10**, 4515 (1998).
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- A. F. Bello, T. van Buuren, J. E. Klepeis, and T. W. Barbee, Jr., *Interfacial electronic charge transfer and density of states in short period Cu/Cr multilayers*, in Applications of Synchrotron Radiation Techniques to Materials Science IV, edited by S. M. Mini, S. R. Stock, D. L. Perry, and L. J. Terminello (Materials Research Society, Warrendale, PA, 1998) p. 285.
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L. Pizzagalli, G. Galli, J. E. Klepeis, and F. Gygi, *Structure and stability of germanium nanoparticles*, Phys. Rev. B **63**, 165324 (2001).

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L. X. Benedict, A. Puzder, A. J. Williamson, J. C. Grossman, G. Galli, J. E. Klepeis, J.-Y. Raty, and O. Pankratov, *Calculation of optical absorption spectra of hydrogenated Si clusters: Bethe-Salpeter equation versus time-dependent local-density approximation*, Phys. Rev. B **68**, 085310 (2003).